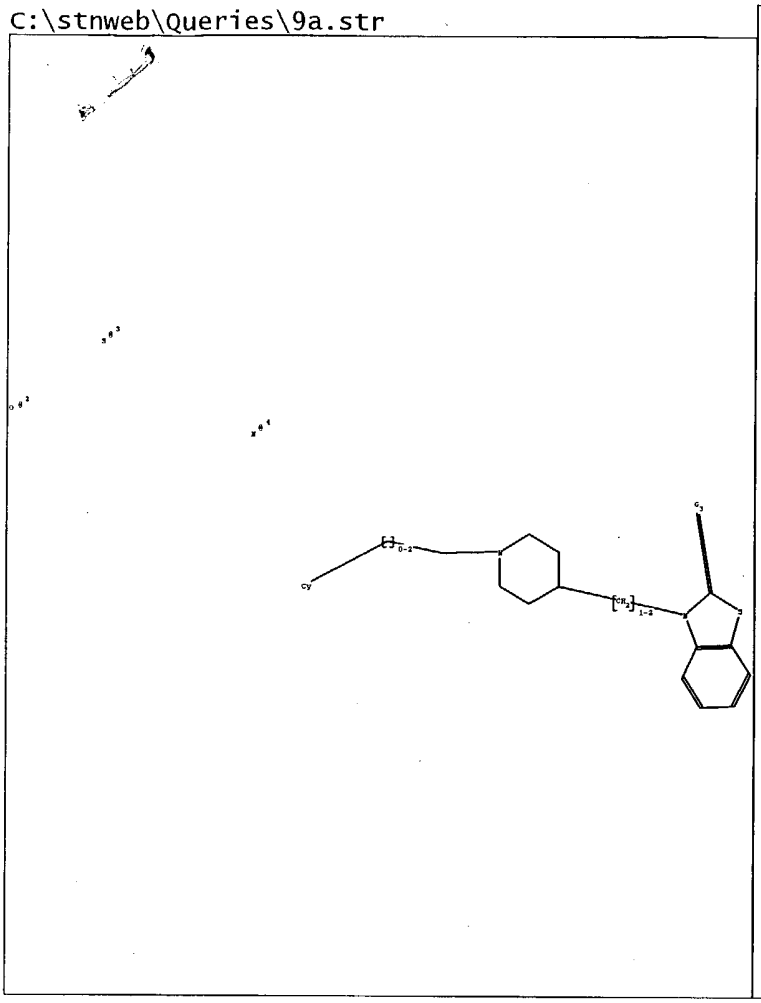
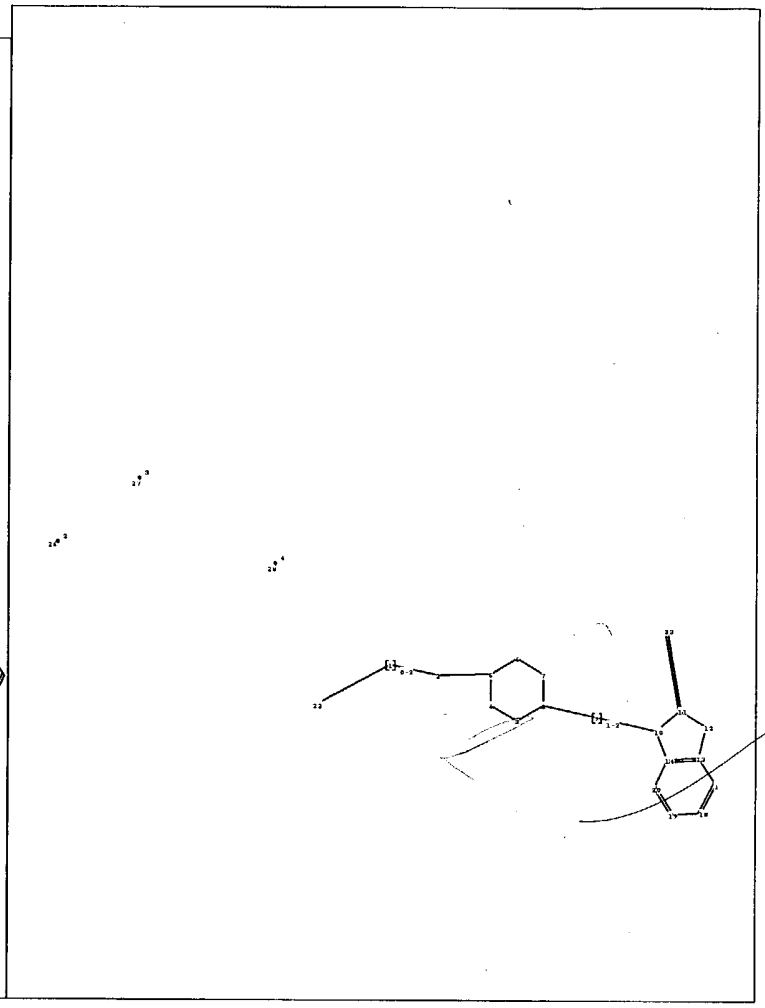
C:\stnweb\Queries\9a.str





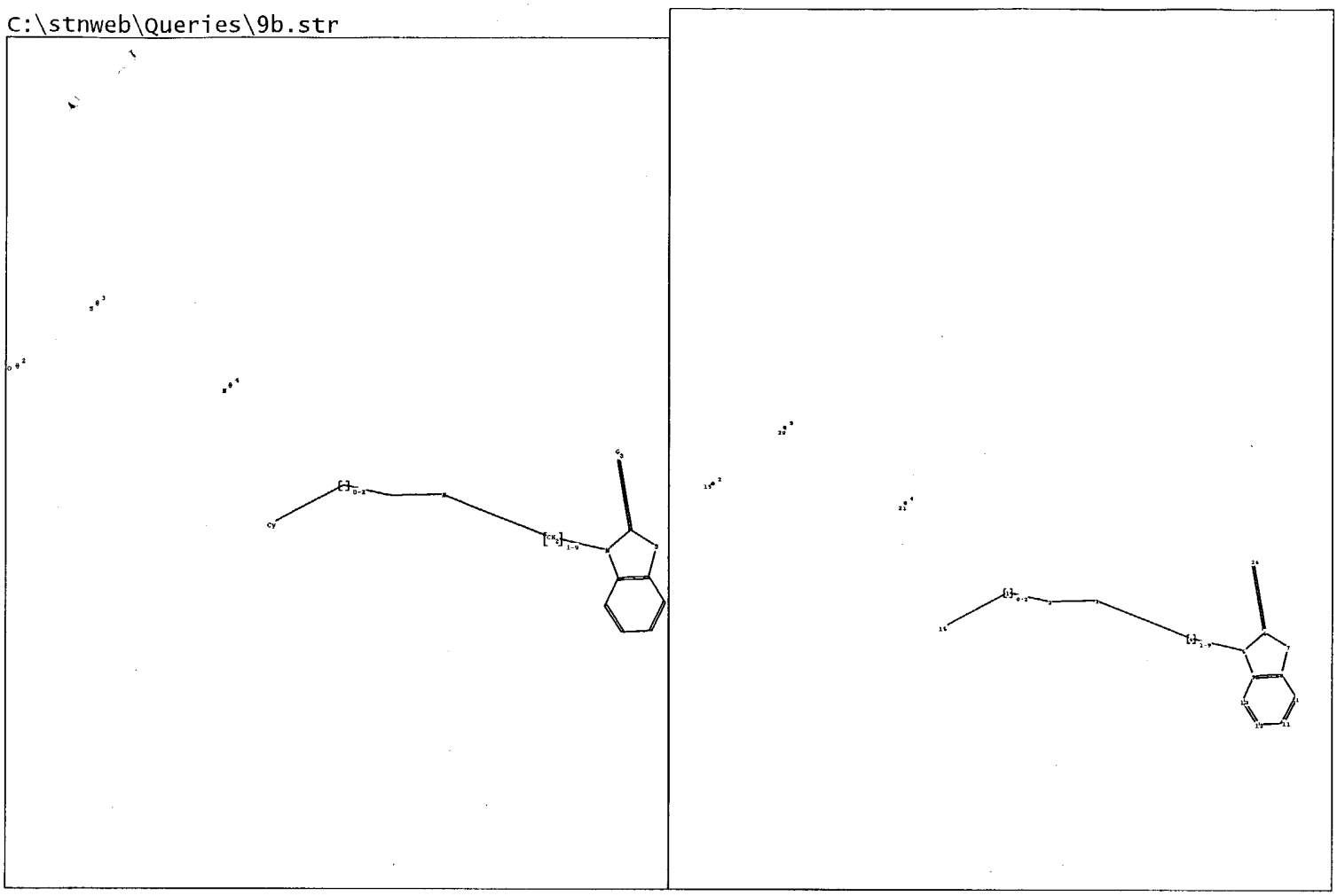
chain nodes :
1 2 9 22 26 27 28 33
ring nodes :
3 4 5 6 7 8 10 11 12 13 14 17 18 19 20
chain bonds :
1-2 1-22 2-5 8-9 9-10 11-33
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8 10-11 10-14 11-12 12-13 13-14 13-17 14-20 17-18
18-19 19-20
exact/norm bonds :
1-22 2-5 3-4 3-8 4-5 5-6 6-7 7-8 10-11 10-14 11-33
exact bonds :
1-2 8-9 9-10 11-12 12-13
normalized bonds :
13-14 13-17 14-20 17-18 18-19 19-20
isolated ring systems :
containing 10 :

G2

G3:[*2],[*3],[*4]

Match level :
1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom 22:Atom 26:CLASS
27:CLASS 28:CLASS 33:CLASS

C:\stnweb\Queries\9b.str



```
chain nodes :
    1  2  3  4  15  19  20  21  26
ring nodes :
    5  6  7  8  9  10  11  12  13
chain bonds :
    1-2  1-15  2-3  3-4  4-5  6-26
ring bonds :
    5-6  5-9  6-7  7-8  8-9  8-10  9-13  10-11  11-12  12-13
exact/norm bonds :
    1-15  2-3  5-6  5-9  6-26
exact bonds :
    1-2  3-4  4-5  6-7  7-8
normalized bonds :
    8-9  8-10  9-13  10-11  11-12  12-13
isolated ring systems :
    containing 5 :


G2

G3:[*2],[*3],[*4]

Match level :
    1:CLASS  2:CLASS  3:Atom  4:CLASS  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
    11:Atom  12:Atom  13:Atom  15:Atom  19:CLASS  20:CLASS  21:CLASS  26:CLASS
```

```
* * * * * * * * * *  Welcome to STN International  * * * * * * * * * *

NEWS 1          Web Page URLs for STN Seminar Schedule - N. America
NEWS 2          "Ask CAS" for self-help around the clock
NEWS 3  Jul 12  BEILSTEIN enhanced with new display and select options,
                resulting in a closer connection to BABS
NEWS 4  AUG 02  IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                fields
NEWS 5  AUG 02  CAplus and CA patent records enhanced with European and Japan
                Patent Office Classifications
NEWS 6  AUG 02  The Analysis Edition of STN Express with Discover!
                (Version 7.01 for Windows) now available
NEWS 7  AUG 27  BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 8  AUG 27  BIOTECHABS/BIOTECHDS: Two new display fields added for legal
                status data from INPADOC
NEWS 9  SEP 01  INPADOC: New family current-awareness alert (SDI) available
NEWS 10 SEP 01  New pricing for the Save Answers for SciFinder Wizard within
                STN Express with Discover!
NEWS 11 SEP 01  New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 12 SEP 14  STN Patent Forum to be held October 13, 2004, in Iselin, NJ
NEWS 13 SEP 27  STANDARDS will no longer be available on STN
NEWS 14 SEP 27  SWETSCAN will no longer be available on STN

NEWS EXPRESS  JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
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  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 20:50:26 ON 19 OCT 2004

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.21       0.21

FILE 'REGISTRY' ENTERED AT 20:50:33 ON 19 OCT 2004
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STRUCTURE FILE UPDATES:   18 OCT 2004  HIGHEST RN 765254-38-4
DICTIONARY FILE UPDATES:  18 OCT 2004  HIGHEST RN 765254-38-4
```

h eb c g cg b cg eb

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

=> s l1
SAMPLE SEARCH INITIATED 20:54:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:54:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.01

L3 18 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 157.94 158.15

FILE 'HCAPLUS' ENTERED AT 20:54:30 ON 19 OCT 2004
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h eb c g cg b cg eb

FILE COVERS 1907 - 19 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 18 Oct 2004 (20041018/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L4 1 L3

=> file req
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 2.36 160.51

FILE 'REGISTRY' ENTERED AT 20:54:37 ON 19 OCT 2004
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DICTIONARY FILE UPDATES: 18 OCT 2004 HIGHEST RN 765254-38-4

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR

=> s l5
SAMPLE SEARCH INITIATED 20:57:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 90 TO ITERATE

100.0% PROCESSED 90 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

h eb c g cg b cg eb

```
PROJECTED ITERATIONS:          1231 TO     2369
PROJECTED ANSWERS:                0 TO        0

L6             0 SEA SSS SAM L5

=> s l5 xfull
COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms.  L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles.  The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:57:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    1714 TO ITERATE

100.0% PROCESSED     1714 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L7             0 SEA SSS FUL L5

=> file reg
COST IN U.S. DOLLARS                                 SINCE FILE      TOTAL
                                                        ENTRY     SESSION
FULL ESTIMATED COST                                    157.94      318.45

FILE 'REGISTRY' ENTERED AT 20:58:31 ON 19 OCT 2004
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DICTIONARY FILE UPDATES:  18 OCT 2004  HIGHEST RN 765254-38-4

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Experimental and calculated property data are now available. For more
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to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L8       STRUCTURE UPLOADED

=> s l8
SAMPLE SEARCH INITIATED 20:59:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       5 TO ITERATE
```

h ebc gcgb cg eb

```
100.0% PROCESSED       5 ITERATIONS                          1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            5 TO      234
PROJECTED ANSWERS:               1 TO       80

L9            1 SEA SSS SAM L8

=> s l8 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 20:59:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    100 TO ITERATE

100.0% PROCESSED     100 ITERATIONS                         18 ANSWERS
SEARCH TIME: 00.00.01

L10           18 SEA SSS FUL L8

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                             155.42     473.87

FILE 'HCAPLUS' ENTERED AT 20:59:24 ON 19 OCT 2004
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FILE COVERS 1907 - 19 Oct 2004  VOL 141 ISS 17
FILE LAST UPDATED: 18 Oct 2004  (20041018/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l10
L11           1 L10

=> file reg
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               2.36     476.23

FILE 'REGISTRY' ENTERED AT 20:59:29 ON 19 OCT 2004
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```

h eb c g cg b cg eb

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STRUCTURE FILE UPDATES: 18 OCT 2004 HIGHEST RN 765254-38-4
DICTIONARY FILE UPDATES: 18 OCT 2004 HIGHEST RN 765254-38-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L12 STRUCTURE UPLOADED

=> d l12
L12 HAS NO ANSWERS
L12 STR

=> s l12
SAMPLE SEARCH INITIATED 21:04:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5 TO 234
PROJECTED ANSWERS: 1 TO 80

L13 1 SEA SSS SAM L12

=> s l12 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:04:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 100 TO ITERATE

100.0% PROCESSED 100 ITERATIONS 26 ANSWERS
SEARCH TIME: 00.00.01

L14 26 SEA SSS FUL L12

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY 158.78 TOTAL SESSION 635.01

FILE 'HCAPLUS' ENTERED AT 21:05:01 ON 19 OCT 2004
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

h eb c g cg b cg eb

FILE COVERS 1907 - 19 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 18 Oct 2004 (20041018/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l14
L15 1 L14

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.36	637.37

FILE 'REGISTRY' ENTERED AT 21:05:06 ON 19 OCT 2004
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DICTIONARY FILE UPDATES: 18 OCT 2004 HIGHEST RN 765254-38-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L16 STRUCTURE UPLOADED

=> s l16
SAMPLE SEARCH INITIATED 21:06:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

h eb c g cg b cg eb

```
FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             0 TO         0
PROJECTED ANSWERS:                0 TO         0

L17           0 SEA SSS SAM L16

=> s l16 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:06:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     11 TO ITERATE

100.0% PROCESSED      11 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L18           0 SEA SSS FUL L16

=>
L19     STRUCTURE UPLOADED

=> s l19
SAMPLE SEARCH INITIATED 21:08:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     10 TO ITERATE

100.0% PROCESSED      10 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:            11 TO       389
PROJECTED ANSWERS:                0 TO         0

L20           0 SEA SSS SAM L19

=> s l19 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:08:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    109 TO ITERATE

100.0% PROCESSED     109 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L21           0 SEA SSS FUL L19

=> d l19
L19 HAS NO ANSWERS
L19             STR

=>
L22     STRUCTURE UPLOADED

=> d l22
L22 HAS NO ANSWERS
L22             STR
```

Page 1-D

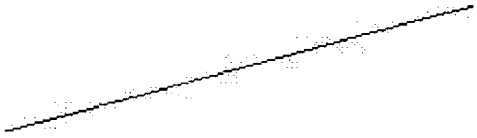
0 22

Page 1-F

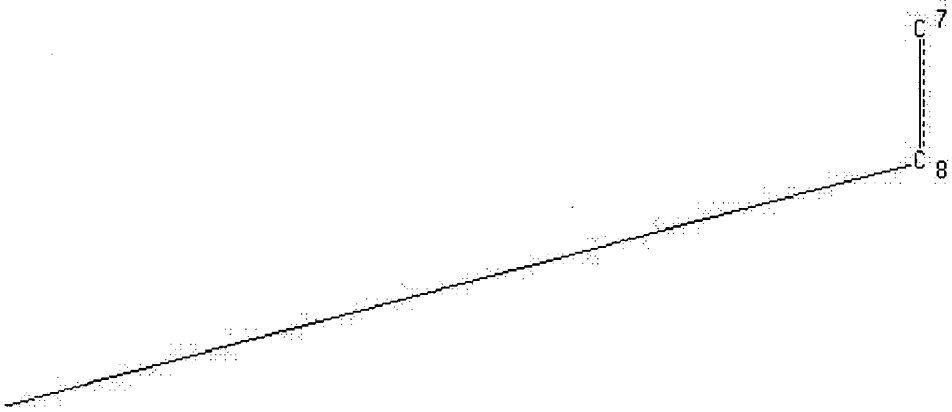
S 23

N 24

Page 1-G

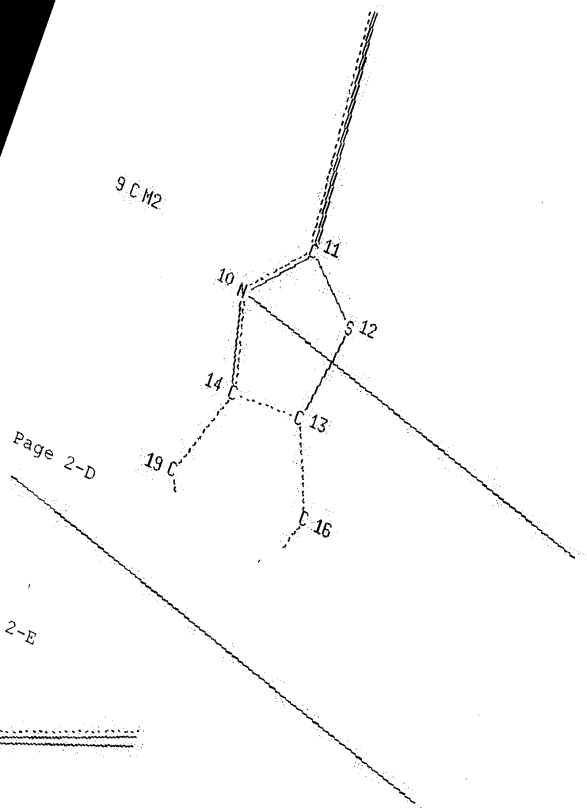


Page 2-A



Page 2-B

h eb c g cg b cg eb



Page 2-D

Page 2-E

Page 2-F

C 1

C4 20

2
C=

Page 2-G

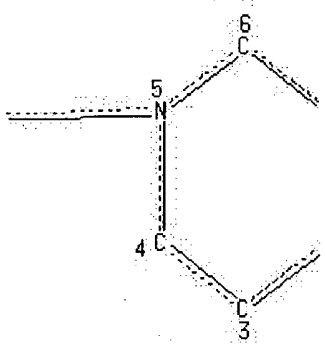
h

eb c

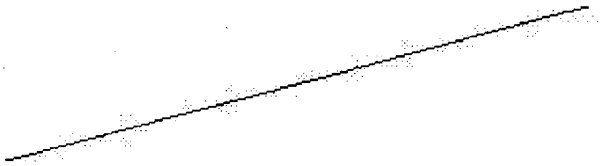
g cg b

cg

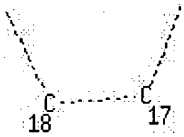
eb



Page 2-H

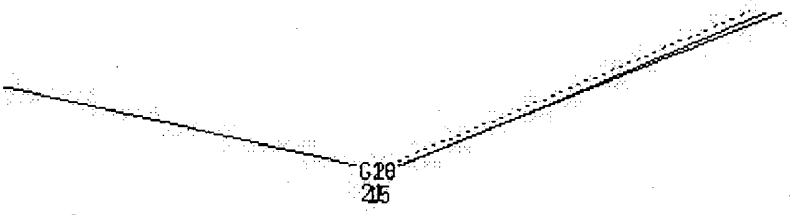


Page 3-A



Page 3-D

Page 3-E



Page 3-F

```
REP G19=(0-2) 1-2 1-20
REP G20=(1-2) 9-8 9-10
VAR G3=22/23/24
NODE ATTRIBUTES:
HCOUNT   IS M2      AT   9
NSPEC    IS C       AT   1
NSPEC    IS C       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS R       AT   7
NSPEC    IS R       AT   8
NSPEC    IS C       AT   9
NSPEC    IS R       AT  10
NSPEC    IS R       AT  11
NSPEC    IS R       AT  12
NSPEC    IS R       AT  13
NSPEC    IS R       AT  14
NSPEC    IS C       AT  15
```

h eb c g cg b cg eb

```
NSPEC   IS R      AT  16
NSPEC   IS R      AT  17
NSPEC   IS R      AT  18
NSPEC   IS R      AT  19
NSPEC   IS C      AT  20
NSPEC   IS C      AT  21
NSPEC   IS C      AT  22
NSPEC   IS C      AT  23
NSPEC   IS C      AT  24
NSPEC   IS C      AT  25
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   1  2  9 22 23 24
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC  10
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE


=> s l22
SAMPLE SEARCH INITIATED 21:15:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      8 TO ITERATE

100.0% PROCESSED       8 ITERATIONS                              3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            8 TO      329
PROJECTED ANSWERS:               3 TO      163

L23           3 SEA SSS SAM L22

=> s l22 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:15:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    165 TO ITERATE

100.0% PROCESSED     165 ITERATIONS                             91 ANSWERS
SEARCH TIME: 00.00.01

L24          91 SEA SSS FUL L22

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               472.14    1109.51

FILE 'HCAPLUS' ENTERED AT 21:15:27 ON 19 OCT 2004
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FILE COVERS 1907 - 19 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 18 Oct 2004 (20041018/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l24
L25 1 L24

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.36	1111.87

FILE 'REGISTRY' ENTERED AT 21:15:37 ON 19 OCT 2004
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STRUCTURE FILE UPDATES: 18 OCT 2004 HIGHEST RN 765254-38-4
DICTIONARY FILE UPDATES: 18 OCT 2004 HIGHEST RN 765254-38-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L26 STRUCTURE UPLOADED

=> s l26
SAMPLE SEARCH INITIATED 21:17:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 100 TO ITERATE

100.0% PROCESSED 100 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:	ONLINE	**COMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	1401 TO	2599
PROJECTED ANSWERS:	1 TO	80

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L27 1 SEA SSS SAM L26

=> s l26 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:17:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1749 TO ITERATE

100.0% PROCESSED 1749 ITERATIONS 58 ANSWERS
SEARCH TIME: 00.00.01

L28 58 SEA SSS FUL L26

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 156.68 1268.55

FILE 'HCAPLUS' ENTERED AT 21:17:48 ON 19 OCT 2004
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FILE COVERS 1907 - 19 Oct 2004 VOL 141 ISS 17
FILE LAST UPDATED: 18 Oct 2004 (20041018/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l28
L29 23 L28

=> s l29 and rocher, j?/au
75 ROCHER, J?/AU
L30 1 L29 AND ROCHER, J?/AU

=> d l30, ibib abs fhitstr, 1

L30 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | Citing References

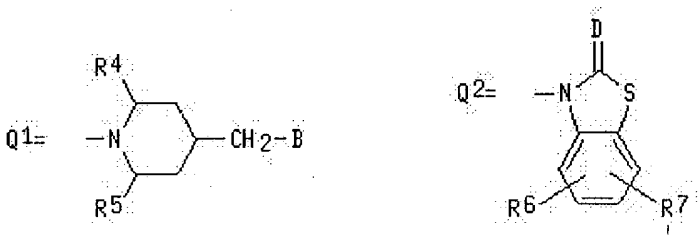
ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): **Rocher, Jean-Philippe**; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama,

h eb c g cg b cg eb

Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607 A	19971105
			WO 1998-JP4973 W	19981104

OTHER SOURCE(S): MARPAT 130:338102
GI



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ-receptors and exhibit small inhibition consts. Ki against σ-1 and/or σ-2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ-ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn.

h . eb c g cg b cg eb

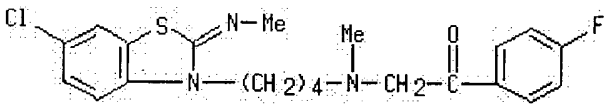
in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT **224443-03-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-03-2 HCAPLUS

CN Ethanone, 2-[[4-[6-chloro-2-(methylimino)-3(2H)-benzothiazolyl]butyl]methylamino]-1-(4-fluorophenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 20:50:26 ON 19 OCT 2004)

FILE 'REGISTRY' ENTERED AT 20:50:33 ON 19 OCT 2004
L1 STRUCTURE UPLOADED
L2 1 S L1
L3 18 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 20:54:30 ON 19 OCT 2004
L4 1 S L3

FILE 'REGISTRY' ENTERED AT 20:54:37 ON 19 OCT 2004
L5 STRUCTURE UPLOADED
L6 0 S L5
L7 0 S L5 FULL

FILE 'REGISTRY' ENTERED AT 20:58:31 ON 19 OCT 2004
L8 STRUCTURE UPLOADED
L9 1 S L8
L10 18 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 20:59:24 ON 19 OCT 2004
L11 1 S L10

FILE 'REGISTRY' ENTERED AT 20:59:29 ON 19 OCT 2004
L12 STRUCTURE UPLOADED

h eb c g cg b cg eb

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L13           1 S L12
L14          26 S L12 FULL

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L15           1 S L14

     FILE 'REGISTRY' ENTERED AT 21:05:06 ON 19 OCT 2004
L16             STRUCTURE UPLOADED
L17           0 S L16
L18           0 S L16 FULL
L19             STRUCTURE UPLOADED
L20           0 S L19
L21           0 S L19 FULL
L22             STRUCTURE UPLOADED
L23           3 S L22
L24          91 S L22 FULL

     FILE 'HCAPLUS' ENTERED AT 21:15:27 ON 19 OCT 2004
L25           1 S L24

     FILE 'REGISTRY' ENTERED AT 21:15:37 ON 19 OCT 2004
L26             STRUCTURE UPLOADED
L27           1 S L26
L28          58 S L26 FULL

     FILE 'HCAPLUS' ENTERED AT 21:17:48 ON 19 OCT 2004
L29          23 S L28
L30           1 S L29 AND ROCHER, J?/AU

=> s l29 not l30
L31          22 L29 NOT L30

=> s l31 and yamabe, h?/au
         210 YAMABE, H?/AU
L32          0 L31 AND YAMABE, H?/AU

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          75 CHAKI, H?/AU
L33          0 L31 AND CHAKI, H?/AU

=> s l31 and saito, k?/au
       10891 SAITO, K?/AU
L34          0 L31 AND SAITO, K?/AU

=> s l31 and abe, m?/au
        5572 ABE, M?/AU
L35          0 L31 AND ABE, M?/AU

=> s l31 and okuyama, m?/au
        1001 OKUYAMA, M?/AU
L36          0 L31 AND OKUYAMA, M?/AU

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     FILE 'REGISTRY' ENTERED AT 20:50:33 ON 19 OCT 2004
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L2            1 S L1
L3           18 S L1 FULL
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h eb c g cg b cg eb

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     FILE 'HCAPLUS' ENTERED AT 20:54:30 ON 19 OCT 2004
L4             1 S L3

     FILE 'REGISTRY' ENTERED AT 20:54:37 ON 19 OCT 2004
L5               STRUCTURE UPLOADED
L6             0 S L5
L7             0 S L5 FULL

     FILE 'REGISTRY' ENTERED AT 20:58:31 ON 19 OCT 2004
L8               STRUCTURE UPLOADED
L9             1 S L8
L10           18 S L8 FULL

     FILE 'HCAPLUS' ENTERED AT 20:59:24 ON 19 OCT 2004
L11            1 S L10

     FILE 'REGISTRY' ENTERED AT 20:59:29 ON 19 OCT 2004
L12              STRUCTURE UPLOADED
L13            1 S L12
L14           26 S L12 FULL

     FILE 'HCAPLUS' ENTERED AT 21:05:01 ON 19 OCT 2004
L15            1 S L14

     FILE 'REGISTRY' ENTERED AT 21:05:06 ON 19 OCT 2004
L16              STRUCTURE UPLOADED
L17            0 S L16
L18            0 S L16 FULL
L19              STRUCTURE UPLOADED
L20            0 S L19
L21            0 S L19 FULL
L22              STRUCTURE UPLOADED
L23            3 S L22
L24           91 S L22 FULL

     FILE 'HCAPLUS' ENTERED AT 21:15:27 ON 19 OCT 2004
L25            1 S L24

     FILE 'REGISTRY' ENTERED AT 21:15:37 ON 19 OCT 2004
L26              STRUCTURE UPLOADED
L27            1 S L26
L28           58 S L26 FULL

     FILE 'HCAPLUS' ENTERED AT 21:17:48 ON 19 OCT 2004
L29           23 S L28
L30            1 S L29 AND ROCHER, J?/AU
L31           22 S L29 NOT L30
L32            0 S L31 AND YAMABE, H?/AU
L33            0 S L31 AND CHAKI, H?/AU
L34            0 S L31 AND SAITO, K?/AU
L35            0 S L31 AND ABE, M?/AU
L36            0 S L31 AND OKUYAMA, M?/AU

=> d l31, ibib abs fhitstr, 1-22

L31  ANSWER 1 OF 22  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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ACCESSION NUMBER:         1999:420020  HCAPLUS
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h eb c g cg b cg eb

DOCUMENT NUMBER: 131:144528
TITLE: Riluzole Series. Synthesis and in Vivo "Antiglutamate" Activity of 6-Substituted-2-benzothiazolamines and 3-Substituted-2-imino-benzothiazolines
AUTHOR(S): Jimonet, Patrick; Audiau, Francois; Barreau, Michel; Blanchard, Jean-Charles; Boireau, Alain; Bour, Yvette; Coleno, Marie-Annick; Doble, Adam; Doerflinger, Gilles; Do Huu, Claudine; Donat, Marie-Helene; Duchesne, Jean Marie; Ganil, Pierre; Gueremy, Claude; Honore, Eliane; Just, Bernard; Kerphirique, Roselyne; Gontier, Sylvie; Hubert, Philippe; Laduron, Pierre M.; Le Blevec, Joseph; Meunier, Mireille; Miquet, Jean-Marie; Nemecek, Conception; Pasquet, Martine; Piot, Odile; Pratt, Jeremy; Rataud, Jean; Reibaud, Michel; Stutzmann, Jean-Marie; Mignani, Serge
CORPORATE SOURCE: Centre de Recherche de Vitry-Alfortville, Rhone-Poulenc S.A. Rhone-Poulenc Rorer, Vitry-sur-Seine, F 94403, Fr.
SOURCE: Journal of Medicinal Chemistry (1999), 42(15), 2828-2843
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
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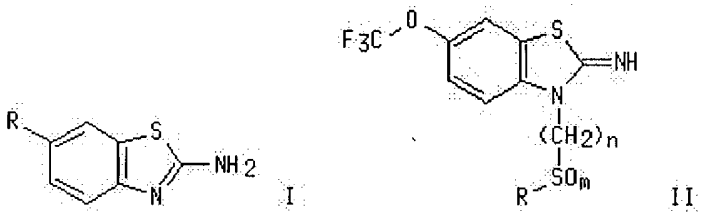
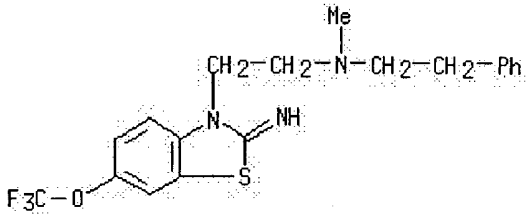


AB Two series of analogs of riluzole, a blocker of excitatory amino acid mediated neurotransmission, have been synthesized: monosubstituted 2-benzothiazolamines and 3-substituted derivs. Of all the compds. prepd. in the first series, only 2-benzothiazolamines bearing alkyl, polyfluoroalkyl, or polyfluoroalkoxy substituents in the 6-position showed potent anticonvulsant activity against administration of glutamic acid in rats. The most active compds. displaying in vivo antiglutamate activity were benzothiazolamines I [R = F3CO (riluzole), F3CCF2O, F3C, F3CCF2] with ED50 values between 2.5 and 3.2 mg/kg i.p. Among the second series of variously substituted benzothiazolines, compds. as active as riluzole or up to 3 times more potent were identified in two series: benzothiazolines bearing a β-dialkylaminoethyl moiety and compds. with an alkylthioalkyl chain and their corresponding sulfoxides and sulfones. The most potent derivs. were II [R = Me, m = 0, n = 2; R = Me, m = 1, n = 2] with ED50 = 1.0 and 1.1 mg/kg i.p., resp.. In addn., i.p. administration of some of the best benzothiazolines protected mice from mortality produced by hypobaric hypoxia.

IT **139362-28-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of benzothiazolamines and iminobenzothiazolines as anticonvulsant agents)
RN 139362-28-0 HCAPLUS

h eb c g cg b cg eb

CN 3(2H)-Benzothiazoleethanamine, 2-imino-N-methyl-N-(2-phenylethyl)-6-(trifluoromethoxy)-, dihydrochloride (9CI) (CA INDEX NAME)



2 HCl

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1999:70442 HCAPLUS
DOCUMENT NUMBER: 130:217160
TITLE: Transition metal complexes with sulfur ligands. Part 135. Electron-rich Fe and Ru complexes with the new trisamine dithiolate ligand 'N3H3S2'-H2 [2,2'-bis(2-mercaptophenylamino)diethylamine]
AUTHOR(S): Sellmann, Dieter; Utz, Juergen; Heinemann, Frank W.
CORPORATE SOURCE: Institut Anorganische Chemie, Universitaet Erlangen, Erlangen, D-91058, Germany
SOURCE: European Journal of Inorganic Chemistry (1999), (2), 341-348
CODEN: EJICFO; ISSN: 1434-1948
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To obtain Fe and Ru complexes which are analogous to [M(L)('NHS4')] and [M(L)('N2H2S3')] complexes ['NHS4'2- = 2,2'-bis(2-mercaptophenylthio)diethylamine(2-), 'N2H2S3'2- = 2,2'-bis(2-mercaptophenylamino)diethylsulfide(2-)] but have electron-richer metal centers, the new pentadentate amine thiolate ligand 'N3H3S2'-H2 [= 2,2'-bis(2-mercaptophenylamino) diethylamine] was synthesized. The dianion 'N3H3S2'2- reacted with FeII salts to give high-spin [Fe('N3H3S2')] (I) [μeff (293 K) = 3.94 μB], which yielded diamagnetic [Fe(CO)('N3H3S2')] (II) upon reaction with CO. II exhibits a low-frequency ν(CO) band (1934 cm^{-1} in THF) indicating an electron-rich Fe center and a strong Fe-CO bond. In spite of this, II readily dissocd. in soln. to I and CO. The reaction of [RuCl2(PPh3)3] with 'N3H3S2'2- yielded [Ru(PPh3)('N3H3S2')] (III), which proved inert with respect to PPh3 substitution but could be methylated at the thiolate donors. The resulting [Ru(PPh3)('N3H3S2'-Me2)]I2 (IV) proved as inert towards substitution as III. IV could reversibly be deprotonated to give [Ru(PPh3)('N3H2S2'-Me2)]I, in the course of which the [RuPN3S2] cores rearrange from CS to C1 symmetry. Reversible protonation/deprotonation was also found with [Ru(NO)('N3H2S2')] (V) which formed from [RuCl3(NO)(PPh3)2] and 'N3H3S2'2- in the presence of one addnl. equiv. of LiOMe. Protonation of V with HBF4 gave [Ru(NO)('N3H3S2')]BF4. The NMR spectra and the x-ray structure anal. of IV (IV.2CH2Cl2: monoclinic, P21/c, a = 1602.7(4), b = 1738.8(4), c = 1695.5(4) Å, β =

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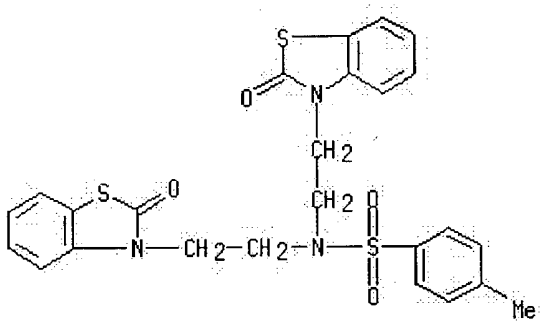
110.67(2)°, V = 4.421(2) nm3, Z = 4, ρc = 1.705 g/cm^3, μ(MoKα) = 2.154, T = 163 K, 7037 obsd. reflections with F0 > 4σ(F0), 620 refined parameters, R1 = 0.0334, wR2 = 0.0918) proved that the [RuPN3S2] cores of III and IV exhibit a CS-sym. meso structure. In all other complexes, however, the [MLN3S2] cores exhibit a C1-sym. structure. It results from the fac-mer coordination mode of the 'N3H3S2'2- ligand and favors the planarity of amide donors when NH functions are reversibly deprotonated.

IT **220961-17-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reactant for prepn. of Fe and Ru complexes with bis(2-mercaptophenylaminoethyl)amine)

RN 220961-17-1 HCAPLUS
CN Benzenesulfonamide, 4-methyl-N,N-bis[2-(2-oxo-3(2H)-benzothiazolyl)ethyl]- (9CI) (CA INDEX NAME)



L31 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1997:189832 HCAPLUS
DOCUMENT NUMBER: 126:186070
TITLE: 3-[[N-Benzoyl-N-[(benzoylamino)methyl]amino]methyl]-6-bromo-2-benzothiazolinone, useful as a plant growth regulator and algicide, and method of its preparation.
INVENTOR(S): Sidoova, Eva; Perjesy, Alexander; Mitterhauszerova, Ludmila; Kralova, Katarina
PATENT ASSIGNEE(S): Univerzita Komenskeho, Slovakia
SOURCE: Slovakia, 3 pp.
CODEN: SLXXFO
DOCUMENT TYPE: Patent
LANGUAGE: Slovak
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SK 278189	B6	19960306	SK 1989-5894	19891018
PRIORITY APPLN. INFO.:			SK 1989-5894	19891018

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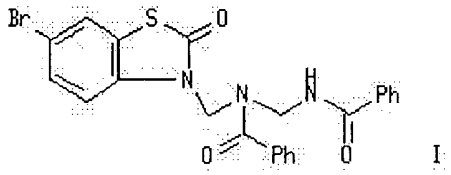


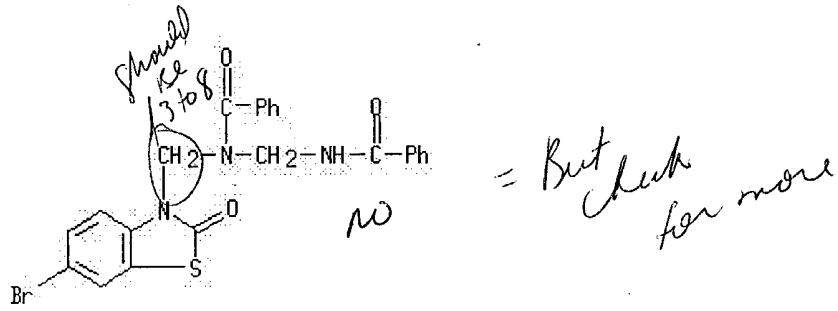
I

AB Title compd. I is prepd. in 72.0% crude yield by reaction of 6-bromo-2-benzothiazolinone with N-(hydroxymethyl)benzamide in refluxing 85% formic acid, and is purified by recrystn. from EtOH using active C. I inhibited growth and chlorophyll synthesis in the green alga Chlorella vulgaris, as well as rooting in corn.

IT **143837-79-0P**, 3-[[N-Benzoyl-N-[(benzoylamino)methyl]amino]methyl]-6-bromo-2-benzothiazolinone
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of [[benzoyl[(benzoylamino)methyl]amino]methyl]bromobenzothiazolinone as plant growth regulator and algicide)

RN 143837-79-0 HCAPLUS

CN Benzamide, N-[(benzoylamino)methyl]-N-[(6-bromo-2-oxo-3(2H)-benzothiazolyl)methyl]- (9CI) (CA INDEX NAME)



L31 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER:	1995:511824 HCAPLUS
DOCUMENT NUMBER:	123:85711
TITLE:	Oxidation-resistant rubber compositions containing benzothiazoline-2-thiones as vulcanization accelerators
INVENTOR(S):	Hatayama, Kazuya
PATENT ASSIGNEE(S):	Bridgestone Corp, Japan
SOURCE:	Jpn. Kokai Tokkyo Koho, 5 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

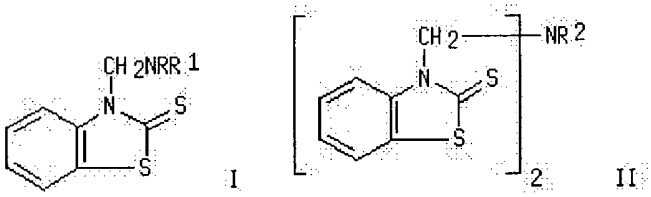
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07041604	A2	19950210	JP 1993-204472	19930728
PRIORITY APPLN. INFO.:			JP 1993-204472	19930728

OTHER SOURCE(S): MARPAT 123:85711

GI

h eb c g cg b cg eb



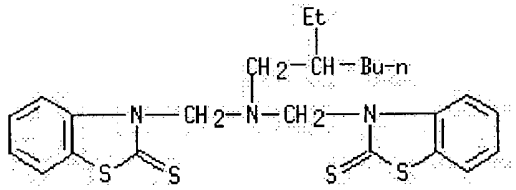
I II

AB The compns. contain vulcanizable rubbers and benzothiazoline-2-thiones I and/or II [R, R1, R2 = H, (un)substituted C1-18 alkyl, aryl, cycloalkyl, Bz, (meth)acryloyl]. Thus, a vulcanizate made from SBR 1500 100, carbon black 50, oil 10, stearic acid 2, antiaging agent 1, Zn flower 3, diphenylguanidine 0.5, and I (R, R1 = Me) 1.35 parts showed good aging resistance in air.

IT **63344-07-0**
RL: CAT (Catalyst use); USES (Uses)
(vulcanization accelerator; oxidn.-resistant rubber compns. contg. benzothiazolinethiones as vulcanization accelerators)

RN 63344-07-0 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3,3'-[[(2-ethylhexyl)imino]bis(methylene)]bis- (9CI) (CA INDEX NAME)



L31 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing Patents

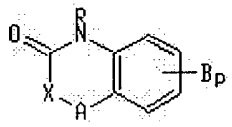
ACCESSION NUMBER: 1993:234044 HCAPLUS
DOCUMENT NUMBER: 118:234044
TITLE: Preparation of N-[(acylamino)ethyl]benzoxazolinones and analogs as nervous system agents
INVENTOR(S): Yous, Said; Lesieur, Isabelle; Depreux, Patrick; Caignard, Daniel Henri; Guardiola, Beatrice; Adam, Gerard; Renard, Pierre
PATENT ASSIGNEE(S): Adir et Compagnie, Fr.
SOURCE: Eur. Pat. Appl., 65 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 506539	A1	19920930	EP 1992-400782	19920324
EP 506539	B1	19970502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE				
FR 2674524	A1	19921002	FR 1991-3538	19910325
FR 2674524	B1	19930521		
US 5240919	A	19930831	US 1992-848373	19920309
CA 2063885	AA	19920926	CA 1992-2063885	19920324
AU 9213112	A1	19921001	AU 1992-13112	19920324
AU 649115	B2	19940512		

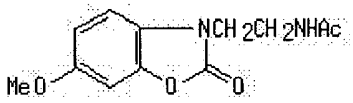
h eb c g cg b cg eb

AT 152448	E	19970515	AT 1992-400782	19920324
ES 2102475	T3	19970801	ES 1992-400782	19920324
JP 05097828	A2	19930420	JP 1992-67453	19920325
JP 07094448	B4	19951011		
US 5300507	A	19940405	US 1993-55665	19930428
US 5322849	A	19940621	US 1993-54596	19930428
US 5322843	A	19940621	US 1993-54720	19930428
US 5326775	A	19940705	US 1993-54604	19930428
US 5386034	A	19950131	US 1993-78001	19930615
US 5436348	A	19950725	US 1994-223176	19940405
PRIORITY APPLN. INFO.:			FR 1991-3538	19910325
			US 1992-848373	19920309
			US 1993-78001	19930615

OTHER SOURCE(S): MARPAT 118:234044
GI



I



II

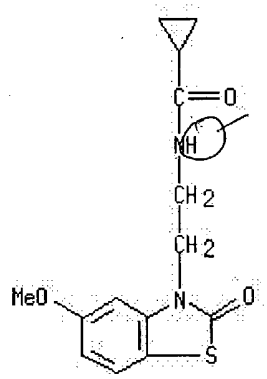
check for more like this

AB Title compds. [I; A = O, S; B = alkoxy, CH2CH2NR1COR2; R = H, alkyl, CH2CH2NR1COR2; R1 = H, alkyl; R2 = H, (halo)alkyl, cycloalkyl, (hetero)aryl, etc.; X = bond, CH2; p = 0, 1] were prepd. as nervous system agents (no data). Thus, 6-methoxybenzoxazolinone was condensed with ClCH2CN and the product reduced to give, after acetylation, title compd. II.

IT **145094-77-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as nervous system agent)

RN 145094-77-5 HCAPLUS

CN Cyclopropanecarboxamide, N-[2-(5-methoxy-2-oxo-3(2H)-benzothiazolyl)ethyl]- (9CI) (CA INDEX NAME)



R3 ≠ H what is claimed
no
is this 103(a)
free amino & protected group

L31 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1993:191730 HCAPLUS
DOCUMENT NUMBER: 118:191730
TITLE: Preparation of benzothiazolinyltropolones for treatment of ischemia.

h eb c g cg b cg eb

INVENTOR(S): McWhoster, William W.; Ito, Noriie; Ozawa, Kazunori; Kushida, Hiroshi; Nomura, Toshiharu; Kunihara, Mineo

PATENT ASSIGNEE(S): Upjohn Co., USA

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04247077	A2	19920903	JP 1991-56252	19910131
CA 2087004	AA	19920301	CA 1991-2087004	19910827
CA 2087004	C	19980421		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
AT 159251	E	19971115	AT 1991-917948	19910827
ES 2109276	T3	19980116	ES 1991-917948	19910827
NO 9300669	A	19930225	NO 1993-669	19930225
US 5594144	A	19970114	US 1995-442710	19950518
US 5703071	A	19971230	US 1995-443972	19950518

PRIORITY APPLN. INFO.:

JP 1990-229536	19900829
JP 1991-56252	19910131
JP 1991-39173	19910208
WO 1991-US5906	19910827
US 1993-975924	19930218

OTHER SOURCE(S): MARPAT 118:191730

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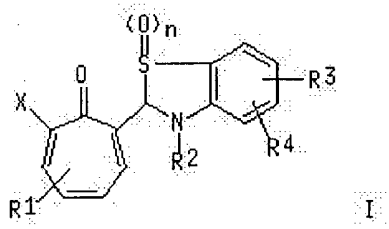


I

AB The title compds. [I; R1 = H, alkyl, (un)substituted aryl; R2 = H, alkyl, etc.; R3, R4 = H, alkyl, halo, OH, alkoxy, etc.; X = OH, alkoxy, etc.; n = 0, 1, 2] were prepd. E.g., 2-[(2-phenylethyl)amino]thiophenol (prepn. given) was refluxed with 2-methoxy-4-isopropyl-7-formyl-2,4,6-cycloheptatrien-1-one in toluene for 17 H to give I [X = MeO, R1 = 5'-iso-Pr, R2 = PhCH2CH2, R3 = R4 = H, n = 0]. At 0.1 mg/Kg i.p. this showed 50% effectiveness in counteracting brain ischemic rats in a learning study using rats.

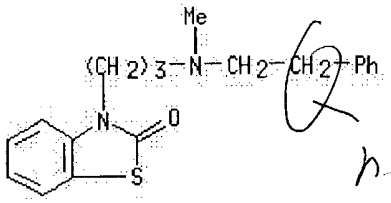
IT **142224-30-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for benzothiazolinyltropolones for treatment of ischemia)

RN 142224-30-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-[methyl(2-phenylethyl)amino]propyl]- (9CI)

h eb c g cg b cg eb

(CA INDEX NAME)

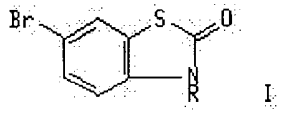


can't just Be ctz
no Benzo

L31 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1992:591740 HCAPLUS
DOCUMENT NUMBER: 117:191740
TITLE: 3-Substituted 6-bromo-2-benzothiazolinones and their antialgal and plant growth regulating activity
AUTHOR(S): Sidoova, E.; Gvozdjakova, A.; Kralova, K.; Mitterhauszerova, L.
CORPORATE SOURCE: Fac. Nat. Sci., Comenius Univ., Bratislava, 842 15, Czech.
SOURCE: Chemical Papers (1992), 46(2), 112-15
CODEN: CHPAEG; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

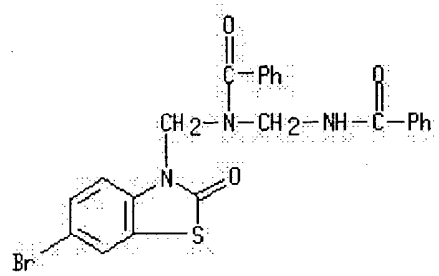


I

AB 6-Bromo-2-benzothiazinone (I, R = H) and its 3-substituted derivs. I (R = Et, Pr, allyl, propargyl, CH2NBzCH2NHBz, Bz, CH2CH2OH, piperidinomethyl) were synthesized. The compds. were tested for plant growth regulating and antialgal activity.

IT **143837-79-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and plant growth regulating and algicidal activity of)

RN 143837-79-0 HCAPLUS
CN Benzamide, N-[(benzoylamino)methyl]-N-[(6-bromo-2-oxo-3(2H)-benzothiazolyl)methyl]- (9CI) (CA INDEX NAME)



no

L31 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

h eb c g cg b cg eb

Full Text | Cited References

ACCESSION NUMBER: 1992:531223 HCAPLUS
DOCUMENT NUMBER: 117:131223
TITLE: Preparation of heterocyclyltropolones as ischemia inhibitors
INVENTOR(S): Ito, Noriie; Kunihara, Mineo; Kushida, Hiroshi; McWhoster, William W.; Nomura, Syunji; Ozawa, Kazunori; Taniguchi, Mikeo; Tsuzuki, Tazuo
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9204338	A1	19920319	WO 1991-US5906	19910827
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW, NO, PL, RO, SD, SU, US				
RW: AT, BE, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN				
JP 04120069	A2	19920421	JP 1990-229536	19900829
AU 9187203	A1	19920330	AU 1991-87203	19910827
AU 651629	B2	19940728		
EP 546102	A1	19930616	EP 1991-917948	19910827
EP 546102	B1	19971015		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 65943	A2	19940829	HU 1993-533	19910827
JP 06509318	T2	19941020	JP 1991-516629	19910827
JP 2512656	B2	19960703		
NO 9300669	A	19930225	NO 1993-669	19930225
PRIORITY APPLN. INFO.:			JP 1990-229536	19900829
			JP 1991-56252	19910131
			JP 1991-39173	19910208
			WO 1991-US5906	19910827

OTHER SOURCE(S): MARPAT 117:131223
GI

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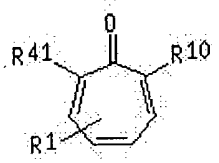

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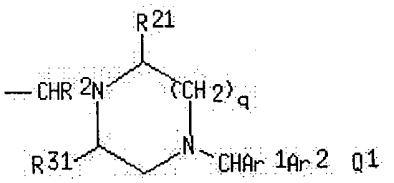
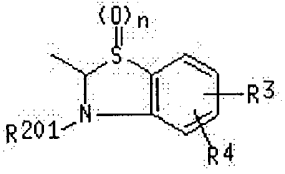
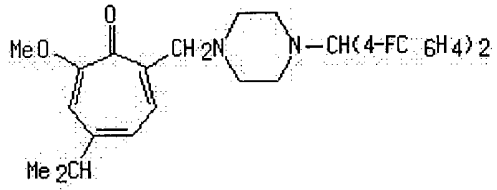






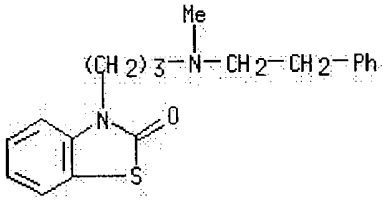
II

AB Title compds. I [R10 = Q1, Q2; R1, R2 = H, C1-5 alkyl, (substituted) aryl, (substituted) hetercyclyl; R3, R4 = H, (substituted) C1-5 alkyl, C7-20 aralkyl, C7-20 aralkyl contg. O, S, or N atoms; halo, OH, C1-5 alkoxy, cyano, etc.; R41 = OR3, OR6, NR7R8, etc.; R6 = H, (substituted) C1-5 alkyl, etc.; R7, R8 = H, (substituted) C1-5 alkyl, C7-20 aralkyl which may contain O, S, or N atoms; NR7R8 = 5-7 membered ring which may contain addnl. O or N atoms; R21, R31 = H, C1-3 alkyl; R201 = H, C1-5 alkyl, C2-20 aralkyl, C6-10 arylsulfonyl, C6-10 arylsulfonyl contg. O, S, or N atoms; Ar1, Ar2 = (substituted) aryl; n = 0-2; q = 1-2], were prepd. Thus, a soln. of 7-chloromethyl-4-isopropyl-2-methoxy-4-isopropyl-2,4,6-cycloheptatrien-1-one (prepn. given), 1-(4,4'-difluorobenzhydryl)piperazine, and Et3N in CHCl3 was refluxed for 20 h to give title compd. II. II had minimal ED of <5 mg/kg i.v. in a ischemic heart/reperfusion test in rats.

IT **142224-30-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for ischemia inhibitors)

RN 142224-30-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-[methyl(2-phenylethyl)amino]propyl]- (9CI) (CA INDEX NAME)



NO

L31 ANSWER 9 OF 22 HCAPLUS. COPYRIGHT 2004 ACS on STN

Full Text | Related References

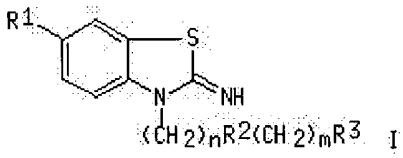
ACCESSION NUMBER: 1992:128911 HCAPLUS
DOCUMENT NUMBER: 116:128911
TITLE: Benzothiazoline derivatives, process for their preparation, and drugs containing them
INVENTOR(S): Gueremy, Claude; Jimonet, Patrick; Mignani, Serge
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer SA, Fr.
SOURCE: PCT Int. Appl., 29 pp.

h eb c g cg b cg eb

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9118892	A1	19911212	WO 1991-FR437	19910531
W: CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
FR 2663029	A1	19911213	FR 1990-7068	19900607
FR 2663029	B1	19920731		
CA 2080005	AA	19911208	CA 1991-2080005	19910531
EP 532602	A1	19930324	EP 1991-910896	19910531
EP 532602	B1	19940803		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 05507918	T2	19931111	JP 1991-510727	19910531
ES 2057901	T3	19941016	ES 1991-910896	19910531
US 5340824	A	19940823	US 1992-938153	19921202
PRIORITY APPLN. INFO.:			FR 1990-7068	19900607
			WO 1991-FR437	19910531

OTHER SOURCE(S): MARPAT 116:128911
GI

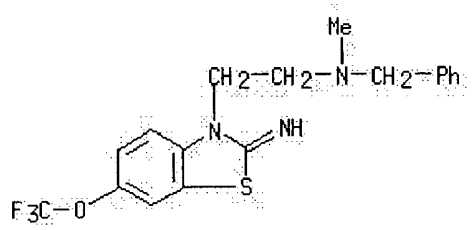


I

AB Benzothiazolines I [R1 = polyfluoroalkoxy; R2 = S, alkylimino, SO, SO2; R3 = Ph, Bz, NR4R5, 1-(phenylalkyl)-4-piperidinyl; R4 = alkyl; R5 = phenylalkyl; n = 1-3; m = 0-3] and salts are prepd. as drugs for treating convulsions, schizophrenia, sleep disorders, cerebral ischemic phenomena, glutamate-related neurol. disorders, Alzheimer's disease (no data). For example, thioetherification of PhCH2NMeCH2CH2SH with 2-[2-(trifluoroacetylimino)-6-(trifluoromethoxy)-3-benzothiazolinyl]ethyl p-toluenesulfonate (prepd. in 3 steps) and subsequent salification gave I (R1 = CF3O, R2 = S, R3 = NMeCH2Ph, n = m = 2) as the dioxalate salt. Nine syntheses and 3 formulations are described.

IT **139362-27-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as neurol. drug)

RN 139362-27-9 HCAPLUS
CN 3(2H)-Benzothiazoleethanamine, 2-imino-N-methyl-N-(phenylmethyl)-6-(trifluoromethoxy)- (9CI) (CA INDEX NAME)



L31 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

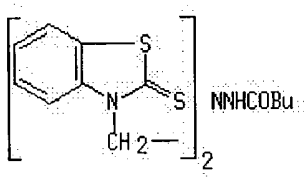
h eb c g cg b cg eb

Full Text | Citing References

ACCESSION NUMBER: 1988:406501 HCAPLUS
DOCUMENT NUMBER: 109:6501
TITLE: Preparation of valeric acid N',N'-bis[(2-thioxo-3-benzothiazolinyl)methyl]hydrazide having antileukemic effect
INVENTOR(S): Holbova, Elena
PATENT ASSIGNEE(S): Czech.
SOURCE: Czech., 2 pp.
CODEN: CZXXA9
DOCUMENT TYPE: Patent
LANGUAGE: Slovak
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 236603	B1	19850515	CS 1981-7170	19811001
PRIORITY APPLN. INFO.:			CS 1981-7170	19811001

GI

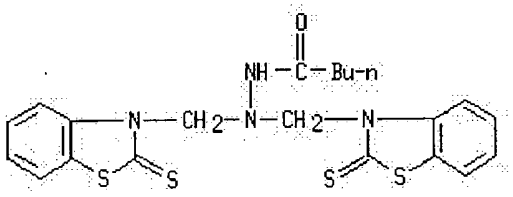


I

AB The title compd. (I) is prepd. by reaction of BuCONHNH2 with 2-mercaptobenzothiazole and CH2O. I is effective against lymphocytic leukemia P388. BuCONHNH2 (11.6 g) was mixed with 33.4 g 2-mercaptobenzothiazole and 200 mL EtOH and the mixt. was heated until it became clear. After addn. of 25 mL 30% formaldehyde, the mixt. was refluxed 10 min and cooled to give 27.4% I. The antileukemic activity against lymphocytic leukemia P388 was tested in female mice. At 50 mg/kg i.p. I increased life span 172%.

IT **76151-51-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as neoplasm inhibitor)

RN 76151-51-4 HCAPLUS
CN Pentanoic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)



L31 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

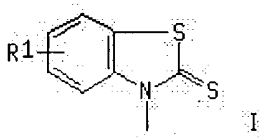
Full Text | Citing References

ACCESSION NUMBER: 1987:87459 HCAPLUS

DOCUMENT NUMBER: 106:87459
TITLE: Aminomethyl derivative of benzothiazolinethione as a lubricant additive
INVENTOR(S): Camenzin, Hugo; Phillips, Emyr
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 203033	A2	19861126	EP 1986-810217	19860520
EP 203033	A3	19890503		
EP 203033	B1	19920311		
R: BE, CH, DE, FR, GB, IT, LI, NL				
CA 1261836	A1	19890926	CA 1986-509580	19860521
BR 8602353	A	19870121	BR 1986-2353	19860522
US 4737302	A	19880412	US 1986-866189	19860522
SU 1498394	A3	19890730	SU 1986-4027563	19860522
JP 61271283	A2	19861201	JP 1986-118988	19860523
JP 07084599	B4	19950913		
US 4803001	A	19890207	US 1988-141165	19880106
US 4810399	A	19890307	US 1988-141175	19880106
PRIORITY APPLN. INFO.:			CH 1985-2199	19850523
			US 1986-866189	19860522

GI

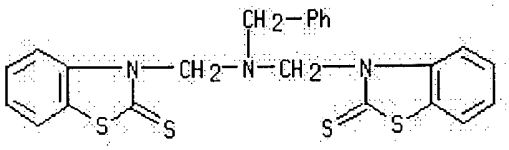


I

AB Lubricating oil additives (e.g., extreme-pressure, antiwear, anticorrosion, and antioxidants) are aminomethyl derivs. of benzothiazoline-2-thiones of structures X-CHR2NR3R4, XCHR2NR3CHR2X, and XCHR2NR3(R5)NR3CHR2X [X = I; R1 = H, C1-12-alkyl, C2-4-alkoxy, C1-24-alkoxycarbonyl, or NO2; R2 = H, C1-12-alkyl, 2-furyl or C1-4-alkyl-2-furyl, C1-4-alkoxy, C1-24-alkoxycarbonyl, or nitrophenyl; R3,R4 = H, C1-20-alkyl, aryl, oxo- or thiono-substituted groups, or alkylphenyl; R3R4 can be a 5- or 6-membered ring; R5 = C5-12-alkylene or heteroatom (O, N, S)-substituted alkylene, C6-15-cycloalkylene, C6-15-arylene (or substituted arylene); N(R3)R5N(R3) can be piperazine-1,4-diyl or substituted piperazine-1,4-diyl]. The additives are typically prepd. from HX (X = I), R2CHO, and R3NHR4 (or R3NH2 or R3NHR5NHR3). A lubricating oil contg. 1 wt.% XCHR2NR3CHR2X (X = I; R1 = R2 = H; R3 = C18H35) had a weld load 200 kg (4-ball test) and wear scar diam. 0.06 mm, compared with 160 kg and 0.90 mm, resp., for the base oil contg. no additive.

IT **63304-34-7**
RL: USES (Uses)
(lubricating oil anticorrosion-antiwear-extreme pressure additive)
RN 63304-34-7 HCAPLUS
CN 2(3H)-Benzothiazolethione, 3,3'-[[(phenylmethyl)imino]bis(methylene)]bis- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

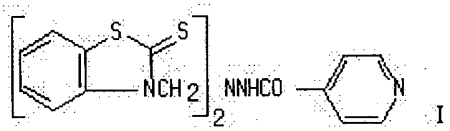


no

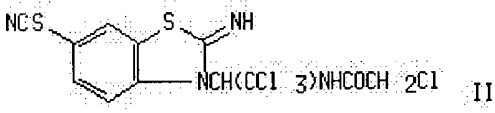
L31 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1983:569092 HCAPLUS
DOCUMENT NUMBER: 99:169092
TITLE: Research in the field of new antituberculotic drugs. Part IV. Derivatives of 2-mercaptobenzothiazole
AUTHOR(S): Odlerova, Z.; Holbova, E.; Sidoova, E.; Gvozdjakova, A.; Mikulasek, S.; Lacova, M.
CORPORATE SOURCE: Vysk. Ustav Prev. Lek., Bratislava, Czech.
SOURCE: Studia Pneumologica et Phtiseologica Cechoslovaca (1983), 43(4), 223-30
CODEN: SPPCAC; ISSN: 0371-2222
DOCUMENT TYPE: Journal
LANGUAGE: Slovak
GI



I



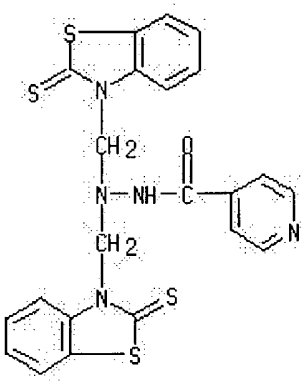
II

AB Of the 325 title compds. screened for tuberculostatic activity against a no. of different species and strains of Mycobacterium, both in vitro and in vivo in mice, the most promising for further study were H-15 (I) [71085-96-6] and SM-363 (II) [87500-73-0].

IT 71085-96-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tuberculostatic activity of)

RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



no

L31 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

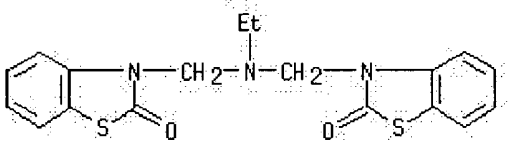
Full Text | Citing References

ACCESSION NUMBER: 1981:208752 HCAPLUS
DOCUMENT NUMBER: 94:208752
TITLE: Benzothiazole compounds. XVII. Preparation and biological activity of Mannich bases with 2-benzothiazolinone
AUTHOR(S): Sutoris, V.; Susoliakova, M.; Holbova, E.; Rada, B.
CORPORATE SOURCE: Fac. Nat. Sci., Komensky Univ., Bratislava, 816 31, Czech.
SOURCE: Chemicke Zvesti (1980), 34(5), 700-5
CODEN: CHZVAN; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:208752

AB Reaction of 2-benzothiazolinone with HCHO and primary amines leads to formation of mono or bis aminomethyl derivs. Reaction of 2-benzothiazolinone with HCHO and secondary amines is also described. Position of the substituents on 2-benzothiazolinone was established by UV and IR spectroscopy. The prepd. compds. are less effective against mycobacteria and viruses than the corresponding derivs. of 2-benzothiazolinethione.

IT **77708-46-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and bactericidal and virucidal activity of)

RN 77708-46-4 HCAPLUS
CN 2(3H)-Benzothiazolone, 3,3'-[(ethylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)



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L31 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

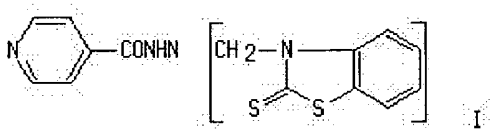
ACCESSION NUMBER: 1981:156915 HCAPLUS
DOCUMENT NUMBER: 94:156915
TITLE: Isonicotinic acid bis[(2-thioxobenzothiazolin-3-yl)methyl]hydrazide
INVENTOR(S): Holbova, Elena; Odlerova, Zelimira
PATENT ASSIGNEE(S): Czech.

h eb c g cg b cg eb

SOURCE: Czech., 4 pp.
CODEN: CZXXA9
DOCUMENT TYPE: Patent
LANGUAGE: Slovak
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 180893	B	19790915	CS 1975-5036	19750716
PRIORITY APPLN. INFO.:			CS 1975-5036	19750716

GI

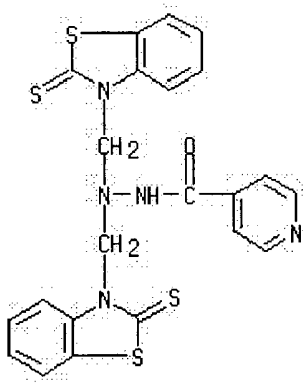


I

AB Refluxing a soln. of equimolar amts. of 2-mercaptobenzothiazole and isonicotinic acid hydrazide in abs. EtOH with dropwise feeding of a double molar amt. of an eq. 37% HCHO soln. gave 50.6% title compd. I. I exhibited in vitro tuberculostatic activity against 5 strains of Mycobacterium tuberculosis and had lower acute toxicity in mice than isoniazide and thiazole. The max. tolerated doses were 1,000 and 500 mg/kg for periods 24 h and 48 h, resp.

IT **71085-96-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and tuberculostatic activity of)

RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)



No

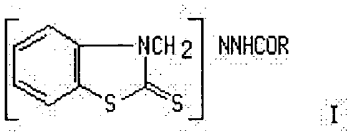
L31 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 1981:30613 HCAPLUS
DOCUMENT NUMBER: 94:30613
TITLE: Benzothiazole compounds. XVI. Preparation and antimycobacterial activity of N',N'-bis[(2-thioxo-3-benzothiazolinyl)methyl]hydrazides
AUTHOR(S): Holbova, E.; Odlerova, Z.

h eb c g cg b cg eb

CORPORATE SOURCE: Inst. Chem., Komensky Univ., Bratislava, 816 50, Czech.
SOURCE: Chemicke Zvesti (1980), 34(3), 399-403
CODEN: CHZVAN; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

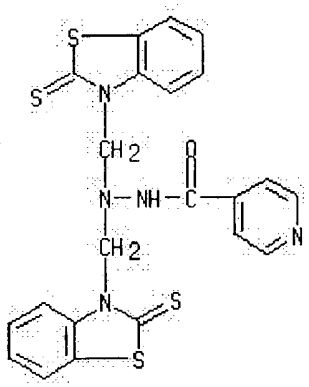


I

AB The reaction of 2-mercaptobenzothiazole with CH2O and RCONHNH2 (R = alkyl, optionally substituted Ph, 4-pyridyl) resulted in bis derivs. of Mannich bases I. The relationship between the formation of bis derivs. and the α effect in hydrazides is explained. I have antimycobacterial activity at 1-50 μg/mL against Mycobacterium tuberculosis H37R4.

IT **71085-96-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and tuberculostatic activity of)

RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)



L31 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1980:215432 HCAPLUS
DOCUMENT NUMBER: 92:215432
TITLE: N-Substituted oxobenzothiazolines
PATENT ASSIGNEE(S): Monsanto Co., USA
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

h eb c g cg b cg eb

JP 54151966	A2	19791129	JP 1979-59801	19790517
US 4227915	A	19801014	US 1978-907233	19780518
PL 117589	B1	19810831	PL 1979-215531	19790512
EP 7161	A1	19800123	EP 1979-300849	19790516
EP 7161	B1	19811021		
R: BE, CH, DE, FR, GB, NL, SE				
DK 7902036	A	19791119	DK 1979-2036	19790517
BR 7903070	A	19791204	BR 1979-3070	19790517
ZA 7902419	A	19800625	ZA 1979-2419	19790517
AU 7947146	A1	19801120	AU 1979-47146	19790517
AU 518626	B2	19811008		
DD 145881	C	19810114	DD 1979-212964	19790517
CS 208500	P	19810915	CS 1979-3437	19790517
CA 1109467	A1	19810922	CA 1979-327946	19790517
IL 57318	A1	19820131	IL 1979-57318	19790517
HU 28040	O	19831128	HU 1979-MO1047	19790517
HU 184662	B	19840928		
PRIORITY APPLN. INFO.:			US 1978-907233	19780518

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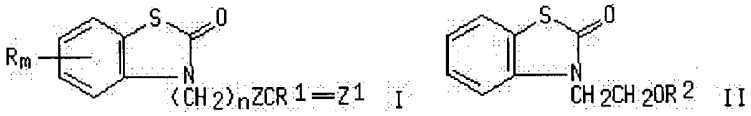


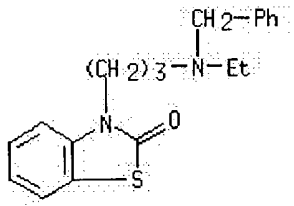
AB Benzothiazolinones I (R = alkyl, alkoxy, halo, CF3, NO2; m = 0-2; n = 1-3; R1 = alkyl, alkenyl, benzyl, Ph, etc.; Z = O, S; Z1 = O, S) (36 compds.) were prepd. I are plant growth regulators. Thus, 2-hydroxybenzothiazole was heated with aq. KOH and ClCH2CH2OH 5 h at 90-100° and 18 h at 25-30° to give 98% II (R2 = H), which was esterified by refluxing with MeNCO and NEt3 in AcOEt 6 h to give 95% II (R2 = CONHMe).

IT **73762-89-7P**

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and plant growth regulating activity of)

RN 73762-89-7 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-[ethyl(phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



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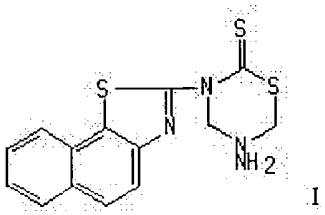
L31 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER:	1979:517174 HCAPLUS
DOCUMENT NUMBER:	91:117174
TITLE:	Antiviral activity of benzothiazole and benzothiazolinethione derivatives in cell cultures
AUTHOR(S):	Rada, B.; Holbova, E.; Mikulasek, S.; Sidoova, E.; Gvozdjakova, A.

h eb c g cg b cg eb

CORPORATE SOURCE: Inst. Virol., Slovak Acad. Sci., Bratislava, 809 39, Czech.
SOURCE: Acta Virologica (English Edition) (1979), 23(3), 203-9
CODEN: AVIRA2; ISSN: 0001-723X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

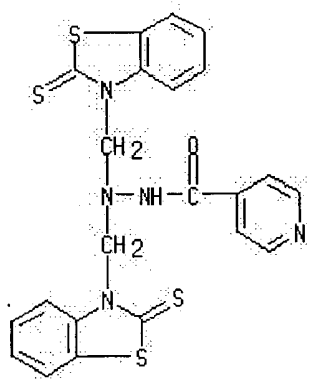


I

AB A total of 58 derivs. of benzothiazole, benzothiazolinethione, and naphthothiazole were tested in vitro against vaccinia virus, Newcastle disease virus (NDV), and western equine encephalomyelitis (WEE). The virucidal activity was largely influenced by the chem. substituents in the mol. Five compds. showed medium and selective activity against vaccinia virus. One compd., 3-(2-α-naphthothiazolyl-5-(4-amino)-tetrahydro-1,3,5-thiadiazine-2-thione (I) [71156-13-3], inhibited both vaccinia and WEE viruses. NDV was inhibited by 2-mercaptobenzothiazole [149-30-4].

IT **71085-96-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(virucidal activity of)

RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)



no

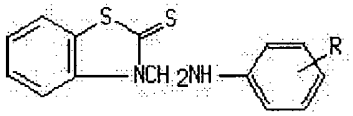
L31 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1977:439353 HCAPLUS
DOCUMENT NUMBER: 87:39353
TITLE: Benzothiazole compounds. X. Mannich reaction of 2-mercaptobenzothiazole with primary amines
AUTHOR(S): Holbova, E.; Sutoris, V.; Blockinger, G.
CORPORATE SOURCE: Inst. Chem., Komensky Univ., Bratislava, Czech.

h eb c g cg b cg eb

SOURCE: Chemicke Zvesti (1976), 30(2), 195-9
CODEN: CHZVAN; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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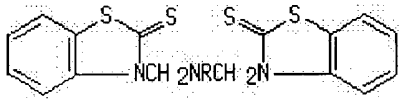
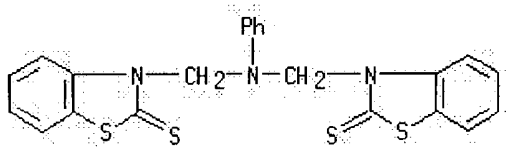


II

AB Aminomethylbenzothiazolinones I (R = p-Me, H, o-NO2) were obtained in 40-94% yield by Mannich reaction of mercaptobenzothiazole with CH2O and RC6H4NH2 10 min at 50-5°. Bis derivs. II [R = cyclohexyl, allyl, PhCH2, Me(CH2)3CHEtCH2, MeOCH2CH2, MeO(CH2)3, Me2CHO(CH2)3] were obtained in 40-80% yields under analogous conditions. Amines with pKB 8-14 led to mono derivs. and amines with pKB 3-5 gave bis derivs.

IT **63304-32-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 63304-32-5 HCAPLUS
CN 2(3H)-Benzothiazolethione, 3,3'-[(phenylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)



no

L31 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN

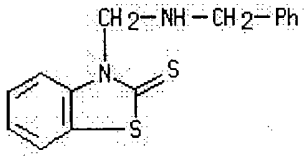
Full Text | Shared References

ACCESSION NUMBER: 1976:17208 HCAPLUS
DOCUMENT NUMBER: 84:17208
TITLE: Spasmolytic activities of aminomethyl derivatives derived from 2-mercaptobenzoxazole and 2-mercaptobenzothiazole
AUTHOR(S): Dhal, P. N.; Nayak, A.
CORPORATE SOURCE: Dep. Chem., Sambalpur Univ., Sambalpur, India
SOURCE: Indian Journal of Pharmacy (1975), 37(4), 92-4
CODEN: IJPAAO; ISSN: 0019-5472
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Mannich reaction of 2-mercaptobenzoxazole and 2-mercaptobenzothiazole with amins gave the (aminomethyl) derivs. (I; X = O, S; R = morpholino, piperidino, pyrrolidino, Et2N, PhCH2NH), which in tests on strips of guinea pig ileum inhibited 50% of the spasm indced by a std. dose of acetylcholine in concn. range of 35-156 μg/ml, and the one by histamine acid phosphate in concn. range of 146-248 μg/ml.

IT **27410-38-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)

h eb c g cg b cg eb

(prepn. and spasmolydic activity of)
RN 27410-38-4 HCAPLUS
CN 2(3H)-Benzothiazolethione, 3-[[(phenylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)

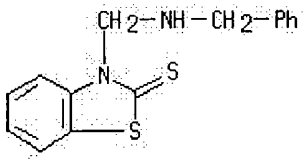


L31 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | Citing References

ACCESSION NUMBER: 1971:87880 HCAPLUS
DOCUMENT NUMBER: 74:87880
TITLE: Michael and Mannich reactions with benzothiazole-2-thiol
AUTHOR(S): Halasa, Adel F.; Smith, George E. P., Jr.
CORPORATE SOURCE: Cent. Res. Lab., Firestone Tire and Rubber Co., Akron, OH, USA
SOURCE: Journal of Organic Chemistry (1971), 36(5), 636-41
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reaction of the anion of benzothiazole-2-thiol (MBT) with activated olefins in the presence of NaH with Michael reaction acceptors produced 3-substituted benzothiazoline-2-thiones. Similarly, the Mannich reaction of MBT anion with HCHO and primary or secondary amines produced the N- (or 3-) substituted benzothiazoline-2-thiones. Possible mechanisms and supporting NMR, ir, and uv data are discussed. The N substitution of MBT anion is discussed within the framework of the oxibase scale which can predict the condition for formation of N products or S products from this ambident anion.

IT **27410-38-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 27410-38-4 HCAPLUS
CN 2(3H)-Benzothiazolethione, 3-[[(phenylmethyl)amino]methyl]- (9CI) (CA INDEX NAME)

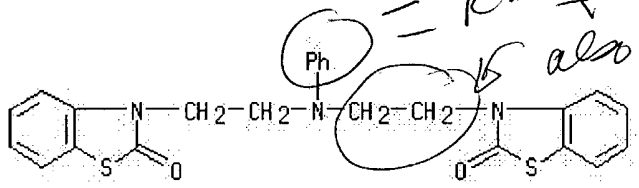


L31 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | Citing References

ACCESSION NUMBER: 1969:115050 HCAPLUS
DOCUMENT NUMBER: 70:115050
TITLE: Benzothiazoline derivatives. II. N-Substituted derivatives of 2-benzothiazolinethione by thiation of the 2-oxo analogs
AUTHOR(S): Sohar, Paul; Denny, George H., Jr.; Babson, Robert D.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Merck and Co., Inc.,

h eb c g cg b cg eb

Rahway, NJ, USA
SOURCE: Journal of Heterocyclic Chemistry (1969), 6(2), 163-74
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:115050
GI For diagram(s), see printed CA Issue.
AB Thiation of the benzoate and acetate esters of 3-(2-hydroxyethyl)-2-benzothiazolinone gave the corresponding thiones. The benzoate was then deblocked to yield 3-(2-hydroxyethyl)-2-benzothiazolinethione (I), a compd. not accessible by direct addn. or substitution. Attempts to introduce a chlorine (or bromine) atom in place of the hydroxyl group in I or its S-isomer, 2-(2-hydroxyethylthio)benzothiazole, gave 2,3-dihydrothiazolo-[2,3-b]benzothiazolium chloride (or bromide) which undergoes dihydrothiazolo ring opening when treated with NaOH or Na2S to give bis[2-(2-benzothiazolinon-3-yl)ethyl]disulfide or bis[2-(2-benzothiazolinethion-3-yl)ethyl]disulfide, resp. 2-Benzothiazolinethione reacted with ethylenimine and with N-phenylethylenimine to give S-substituted derivs. Addn. to vinyl butyl ether gave the expected N-substituted deriv. which was found to undergo removal of the butoxyethyl group when subjected to conventional conditions for ether cleavage.
IT **22274-86-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 22274-86-8 HCAPLUS
CN 2-Benzothiazolinone, 3,3'-[(phenylimino)diethylene]bis- (8CI) (CA INDEX NAME)



= R3 ≠ Ph but ask of prof. group
also no
103(a) = no

L31 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2004 ACS on STN
Full Text | Citing References
ACCESSION NUMBER: 1960:128861 HCAPLUS
DOCUMENT NUMBER: 54:128861
ORIGINAL REFERENCE NO.: 54:24664h-i,24665a-c
TITLE: 2-Mercaptobenzothiazole in Mannich reactions. I. Synthesis, properties, and structure of Mannich bases
AUTHOR(S): Stavrovskaya, V. I.; Kolosova, M. O.
SOURCE: Zhurnal Obshchei Khimii (1960), 30, 689-94
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:128861
AB The Mannich bases from 2-mercaptobenzothiazole were unstable in aq. alkalies or acids or at elevated temps. Reaction of 5 ml. formalin (I) with 8.4 g. 2-mercaptobenzothiazole (II) in Me2CO gave 98% 3-piperidinomethylbenzothiazole-2-thione, m. 159-61°. Similarly were prepd. 3-morpholinomethylbenzothiazolyl-2-thione (III), m. 147-8°, and 3-diethylaminomethylbenzothiazolyl-2-thione, m. 90° (Brit. 377,253, CA 27, 4133). Reaction of HOCH2CH2NH2 with I and II in MeOH gave 57.7% N,N-bis(methylbenzothiazolyl-2-thione)aminoethanol, m. 130°. II and PhNH2 in EtOH with I gave 88% 3-anilinomethylbenzothiazolyl-2-thione (IIIa), m. 105-7°.

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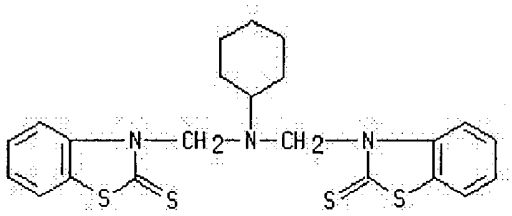
Cyclohexylamine (IIIb) similarly gave 54.5% N,N-bis(methylbenzothiazolyl-2-thione)cyclohexylamine, m. 164-7°. Reaction of 16.7 g. II and 10 ml. I with 20 g. IIIb in EtOH gave 56% II cyclohexylammonium salt, m. 153-5°. III formed an HCl salt, m. 130-2° (open tube), 148° (sealed tube). All the bases were cleaved to mercaptobenzothiazole by 10% HCl or aq. AcOH. II and I in hot EtOH gave 96.5% 3-hydroxymethylbenzothiazolyl-2-thione (IV), m. 128-30°. This and PhNH2 gave IIIa; similarly were run reactions with other amines to yield the above described Mannich bases (m.ps. shown in parentheses): morpholine (147-9°), Et2NH (88°), piperidine (157-8°). IV and IIIb gave the Schiff base, m. 157-8°. IV and SOCl2 gave N-chloromethylbenzothiazolyl-2-thione, m. 123-5°, which with Zn dust in AcOH gave 71% N-methylbenzothiazolyl-2-thione, m. 88°.

IT **102757-22-2**, 2-Benzothiazolinethione, 3,3'-[(cyclohexylimino)dimethylene]bis-
(prepn. of)
RN 102757-22-2 HCAPLUS
CN 2(3H)-Benzothiazolethione, 3,3'-[(cyclohexylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)



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L3 18 S L1 FULL

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L4 1 S L3

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L5 STRUCTURE UPLOADED
L6 0 S L5
L7 0 S L5 FULL

FILE 'REGISTRY' ENTERED AT 20:58:31 ON 19 OCT 2004
L8 STRUCTURE UPLOADED
L9 1 S L8
L10 18 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 20:59:24 ON 19 OCT 2004
L11 1 S L10

FILE 'REGISTRY' ENTERED AT 20:59:29 ON 19 OCT 2004
L12 STRUCTURE UPLOADED
L13 1 S L12

h eb c g cg b cg eb

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L24          91 S L22 FULL

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L29          23 S L28
L30           1 S L29 AND ROCHER, J?/AU
L31          22 S L29 NOT L30
L32           0 S L31 AND YAMABE, H?/AU
L33           0 S L31 AND CHAKI, H?/AU
L34           0 S L31 AND SAITO, K?/AU
L35           0 S L31 AND ABE, M?/AU
L36           0 S L31 AND OKUYAMA, M?/AU

=> s l28/thu
            23 L28
        627560 THU/RL
L37          6 L28/THU
                 (L28 (L) THU/RL)

=> s l37 and nerve
        224970 NERVE
         42386 NERVES
        238102 NERVE
                 (NERVE OR NERVES)
L38          1 L37 AND NERVE

=> d l38, ibib abs fhitstr, 1

L38  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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ACCESSION NUMBER:          1999:311193  HCAPLUS
DOCUMENT NUMBER:           130:338102
TITLE:                     Preparation of N-(aminoalkyl)- or N-(1-
                           piperidinylmethyl)benzothiazoline derivatives as
                           ligands for sigma-receptor
INVENTOR(S):               Rocher, Jean-Philippe; Yamabe, Haruko; Chaki,
                           Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama,
                           Masahiro
```

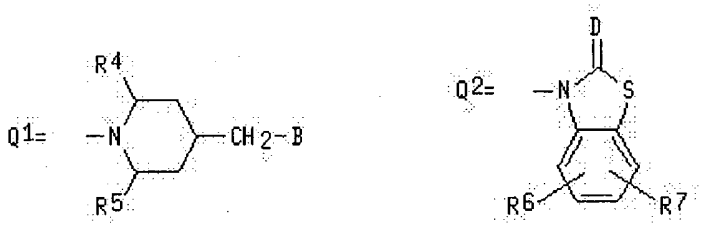
h eb c g cg b cg eb

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104
W: CA, CN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1043319	A1	20001011	EP 1998-951687	19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11217377	A2	19990810	JP 1998-314459	19981105
PRIORITY APPLN. INFO.:			JP 1997-302607 A	19971105
			WO 1998-JP4973 W	19981104

OTHER SOURCE(S): MARPAT 130:338102
GI



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ-receptors and exhibit small inhibition consts. Ki against σ-1 and/or σ-2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by **nerve**-regulating effect of σ-ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give

h eb c g cg b cg eb

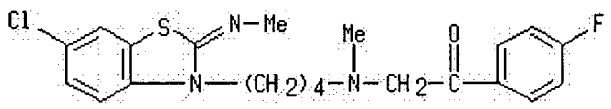
1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT **224443-03-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-03-2 HCAPLUS

CN Ethanone, 2-[[4-[6-chloro-2-(methylimino)-3(2H)-benzothiazolyl]butyl]methylamino]-1-(4-fluorophenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 18 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 20:54:30 ON 19 OCT 2004
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FILE 'REGISTRY' ENTERED AT 20:54:37 ON 19 OCT 2004
L5 STRUCTURE UPLOADED
L6 0 S L5
L7 0 S L5 FULL

FILE 'REGISTRY' ENTERED AT 20:58:31 ON 19 OCT 2004
L8 STRUCTURE UPLOADED
L9 1 S L8
L10 18 S L8 FULL

FILE 'HCAPLUS' ENTERED AT 20:59:24 ON 19 OCT 2004
L11 1 S L10

FILE 'REGISTRY' ENTERED AT 20:59:29 ON 19 OCT 2004
L12 STRUCTURE UPLOADED
L13 1 S L12

h eb c g cg b cg eb

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L14          26 S L12 FULL

     FILE 'HCAPLUS' ENTERED AT 21:05:01 ON 19 OCT 2004
L15           1 S L14

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L16             STRUCTURE UPLOADED
L17           0 S L16
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L20           0 S L19
L21           0 S L19 FULL
L22             STRUCTURE UPLOADED
L23           3 S L22
L24          91 S L22 FULL

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L25           1 S L24

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L26             STRUCTURE UPLOADED
L27           1 S L26
L28          58 S L26 FULL

     FILE 'HCAPLUS' ENTERED AT 21:17:48 ON 19 OCT 2004
L29          23 S L28
L30           1 S L29 AND ROCHER, J?/AU
L31          22 S L29 NOT L30
L32           0 S L31 AND YAMABE, H?/AU
L33           0 S L31 AND CHAKI, H?/AU
L34           0 S L31 AND SAITO, K?/AU
L35           0 S L31 AND ABE, M?/AU
L36           0 S L31 AND OKUYAMA, M?/AU
L37           6 S L28/THU
L38           1 S L37 AND NERVE

=> d l37, ibib abs fhitstr, 1-6

L37  ANSWER 1 OF 6  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Other References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9923083	A1	19990514	WO 1998-JP4973	19981104

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W: CA, CN, KR, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
EP 1043319 A1 20001011 EP 1998-951687 19981104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI
JP 11217377 A2 19990810 JP 1998-314459 19981105
PRIORITY APPLN. INFO.: JP 1997-302607 A 19971105
WO 1998-JP4973 W 19981104
OTHER SOURCE(S): MARPAT 130:338102
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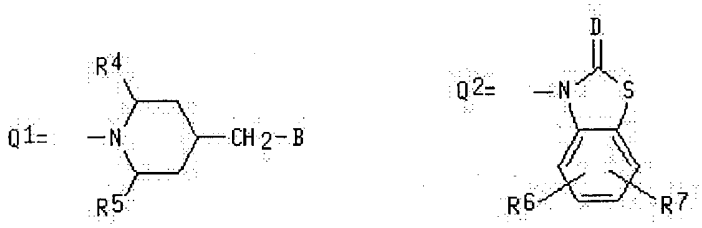

AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ-receptors and exhibit small inhibition consts. Ki against σ-1 and/or σ-2 receptors, are prepd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ-ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H3]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT **224443-03-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic**

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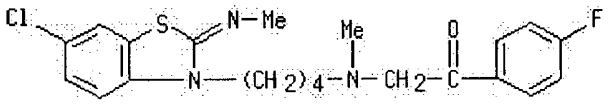
use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-03-2 HCAPLUS
CN Ethanone, 2-[[4-[6-chloro-2-(methylimino)-3(2H)-benzothiazolyl]butyl]methylamino]-1-(4-fluorophenyl)-, dihydrochloride (9CI) (CA INDEX NAME)



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REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1988:406501 HCAPLUS
DOCUMENT NUMBER: 109:6501
TITLE: Preparation of valeric acid N',N'-bis[(2-thioxo-3-benzothiazolinyl)methyl]hydrazide having antileukemic effect
INVENTOR(S): Holbova, Elena
PATENT ASSIGNEE(S): Czech.
SOURCE: Czech., 2 pp.
CODEN: CZXXA9
DOCUMENT TYPE: Patent
LANGUAGE: Slovak
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 236603	B1	19850515	CS 1981-7170	19811001
PRIORITY APPLN. INFO.:			CS 1981-7170	19811001

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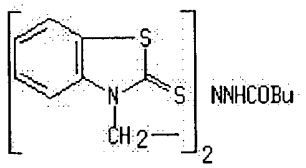

I

AB The title compd. (I) is prepd. by reaction of BuCONHNH2 with 2-mercaptobenzothiazole and CH2O. I is effective against lymphocytic leukemia P388. BuCONHNH2 (11.6 g) was mixed with 33.4 g 2-mercaptobenzothiazole and 200 mL EtOH and the mixt. was heated until it became clear. After addn. of 25 mL 30% formaldehyde, the mixt. was refluxed 10 min and cooled to give 27.4% I. The antileukemic activity against lymphocytic leukemia P388 was tested in female mice. At 50 mg/kg i.p. I increased life span 172%.

IT 76151-51-4P

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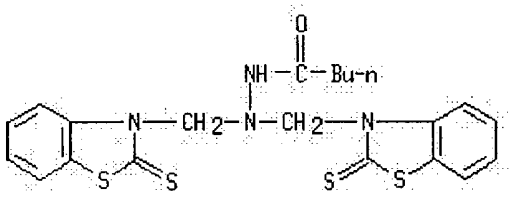
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as neoplasm inhibitor)

RN 76151-51-4 HCAPLUS

CN Pentanoic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)



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L37 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | CAPLUS References

ACCESSION NUMBER: 1983:569092 HCAPLUS
DOCUMENT NUMBER: 99:169092
TITLE: Research in the field of new antituberculotic drugs. Part IV. Derivatives of 2-mercaptobenzothiazole
AUTHOR(S): Odlerova, Z.; Holbova, E.; Sidoova, E.; Gvozdjakova, A.; Mikulasek, S.; Lacova, M.
CORPORATE SOURCE: Vysk. Ustav Prev. Lek., Bratislava, Czech.
SOURCE: Studia Pneumologica et Phtiseologica Cechoslovaca (1983), 43(4), 223-30
CODEN: SPPCAC; ISSN: 0371-2222
DOCUMENT TYPE: Journal
LANGUAGE: Slovak
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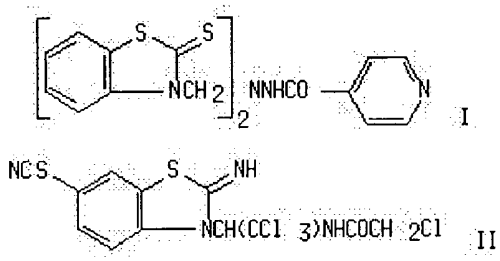

I

II

AB Of the 325 title compds. screened for tuberculostatic activity against a no. of different species and strains of Mycobacterium, both in vitro and in vivo in mice, the most promising for further study were H-15 (I) [71085-96-6] and SM-363 (II) [87500-73-0].

IT **71085-96-6**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(tuberculostatic activity of)

RN 71085-96-6 HCAPLUS

CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)

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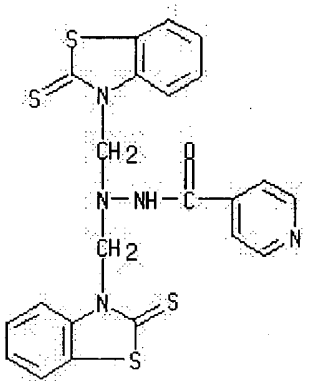


16

L37 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

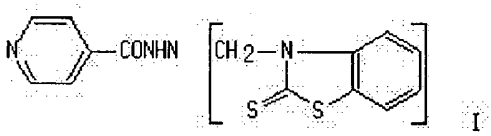
Full Text | Refs & References

ACCESSION NUMBER: 1981:156915 HCAPLUS
DOCUMENT NUMBER: 94:156915
TITLE: Isonicotinic acid bis[(2-thioxobenzothiazolin-3-yl)methyl]hydrazide
INVENTOR(S): Holbova, Elena; Odlerova, Zelimira
PATENT ASSIGNEE(S): Czech.
SOURCE: Czech., 4 pp.
CODEN: CZXXA9
DOCUMENT TYPE: Patent
LANGUAGE: Slovak
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CS 180893	B	19790915	CS 1975-5036	19750716

PRIORITY APPLN. INFO.: CS 1975-5036 19750716

GI

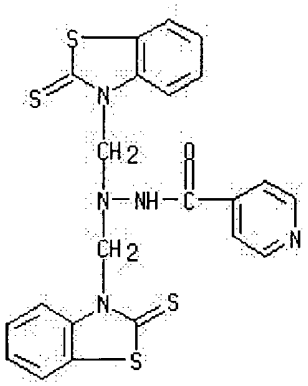


I

AB Refluxing a soln. of equimolar amts. of 2-mercaptobenzothiazole and isonicotinic acid hydrazide in abs. EtOH with dropwise feeding of a double molar amt. of an eq. 37% HCHO soln. gave 50.6% title compd. I. I exhibited in vitro tuberculostatic activity against 5 strains of Mycobacterium tuberculosis and had lower acute toxicity in mice than isoniazide and thiazole. The max. tolerated doses were 1,000 and 500 mg/kg for periods 24 h and 48 h, resp.

IT **71085-96-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and tuberculostatic activity of)
RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

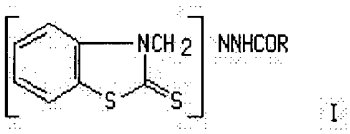


no

L37 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

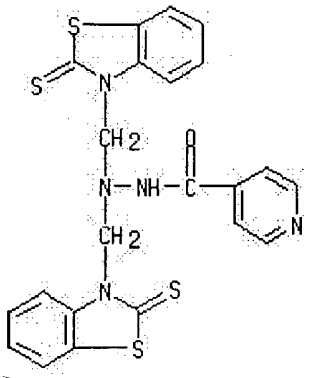
ACCESSION NUMBER: 1981:30613 HCAPLUS
DOCUMENT NUMBER: 94:30613
TITLE: Benzothiazole compounds. XVI. Preparation and antimycobacterial activity of N',N'-bis[(2-thioxo-3-benzothiazolinyl)methyl]hydrazides
AUTHOR(S): Holbova, E.; Odlerova, Z.
CORPORATE SOURCE: Inst. Chem., Komensky Univ., Bratislava, 816 50, Czech.
SOURCE: Chemicke Zvesti (1980), 34(3), 399-403
CODEN: CHZVAN; ISSN: 0366-6352
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The reaction of 2-mercaptobenzothiazole with CH2O and RCONHNH2 (R = alkyl, optionally substituted Ph, 4-pyridyl) resulted in bis derivs. of Mannich bases I. The relationship between the formation of bis derivs. and the α effect in hydrazides is explained. I have antimycobacterial activity at 1-50 μg/mL against Mycobacterium tuberculosis H37R4.

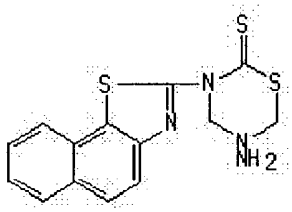
IT **71085-96-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and tuberculostatic activity of)
RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)



L37 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1979:517174 HCAPLUS
DOCUMENT NUMBER: 91:117174
TITLE: Antiviral activity of benzothiazole and benzothiazolinethione derivatives in cell cultures
AUTHOR(S): Rada, B.; Holbova, E.; Mikulasek, S.; Sidoova, E.; Gvozdjakova, A.
CORPORATE SOURCE: Inst. Virol., Slovak Acad. Sci., Bratislava, 809 39, Czech.
SOURCE: Acta Virologica (English Edition) (1979), 23(3), 203-9
CODEN: AVIRA2; ISSN: 0001-723X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



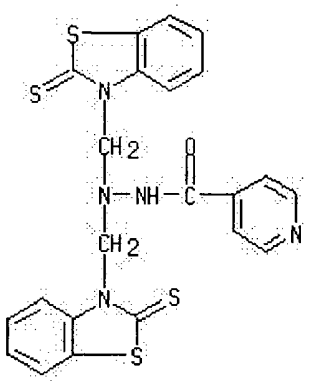
I

AB A total of 58 derivs. of benzothiazole, benzothiazolinethione, and naphthothiazole were tested in vitro against vaccinia virus, Newcastle disease virus (NDV), and western equine encephalomyelitis (WEE). The virucidal activity was largely influenced by the chem. substituents in the mol. Five compds. showed medium and selective activity against vaccinia virus. One compd., 3-(2-α-naphthothiazolyl-5-(4-amino)-tetrahydro-1,3,5-thiadiazine-2-thione (I) [71156-13-3], inhibited both vaccinia and WEE viruses. NDV was inhibited by 2-mercaptobenzothiazole [149-30-4].

IT **71085-96-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **THU (Therapeutic use)**; BIOL (Biological study); USES (Uses)
(virucidal activity of)

RN 71085-96-6 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2,2-bis[(2-thioxo-3(2H)-benzothiazolyl)methyl]hydrazide (9CI) (CA INDEX NAME)

h eb c g cg b cg eb



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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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This file supports REGistRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L3 18 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 20:54:30 ON 19 OCT 2004
L4 1 S L3

FILE 'REGISTRY' ENTERED AT 20:54:37 ON 19 OCT 2004
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L6 0 S L5
L7 0 S L5 FULL

h eb c g cg b cg eb

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L10          18 S L8 FULL

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L11           1 S L10

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L13           1 S L12
L14          26 S L12 FULL

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L18           0 S L16 FULL
L19             STRUCTURE UPLOADED
L20           0 S L19
L21           0 S L19 FULL
L22             STRUCTURE UPLOADED
L23           3 S L22
L24          91 S L22 FULL

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L26             STRUCTURE UPLOADED
L27           1 S L26
L28          58 S L26 FULL

     FILE 'HCAPLUS' ENTERED AT 21:17:48 ON 19 OCT 2004
L29          23 S L28
L30           1 S L29 AND ROCHER, J?/AU
L31          22 S L29 NOT L30
L32           0 S L31 AND YAMABE, H?/AU
L33           0 S L31 AND CHAKI, H?/AU
L34           0 S L31 AND SAITO, K?/AU
L35           0 S L31 AND ABE, M?/AU
L36           0 S L31 AND OKUYAMA, M?/AU
L37           6 S L28/THU
L38           1 S L37 AND NERVE

     FILE 'CAOLD' ENTERED AT 21:22:37 ON 19 OCT 2004

=> s l28
L39           1 L28

=> d l39, all, i

L39  ANSWER 1 OF 1  CAOLD  COPYRIGHT 2004 ACS on STN
AN   CA54:24664i  CAOLD
TI   2-mercaptobenzothiazole in Mannich reactions - (I) synthesis, properties,
     and structure of Mannich bases
AU   Stavrovskaya, V. I.; Kolosova, M. O.
IT   3161-57-7   5392-35-8   6957-11-5  22075-92-9  27410-41-9  37437-20-0
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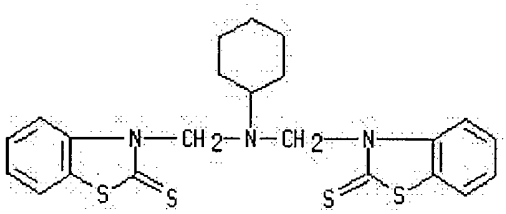
41526-42-5 100722-54-1 **102757-22-2** **112298-86-9** 117866-31-6

=> fil reg; d acc 102757-22-2; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:22:52 ON 19 OCT 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 102757-22-2 REGISTRY
CN 2(3H)-Benzothiazolethione, 3,3'-[(cyclohexylimino)bis(methylene)]bis- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Benzothiazolinethione, 3,3'-[(cyclohexylimino)dimethylene]bis- (6CI)
MF C22 H23 N3 S4
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: USES (Uses)
RL.NP Roles from non-patents: NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

FILE 'CAOLD' ENTERED AT 21:22:52 ON 19 OCT 2004

=> fil reg; d acc 112298-86-9; fil CAOLD

FILE 'REGISTRY' ENTERED AT 21:22:56 ON 19 OCT 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 112298-86-9 REGISTRY
CN 2-Benzothiazolinethione, 3,3'-[(2-hydroxyethylimino)dimethylene]bis- (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H17 N3 O S4
SR CAOLD
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)

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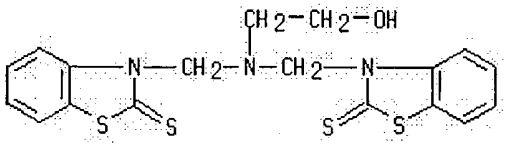

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
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